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Spin currents in thermodynamic equilibrium: The challenge of discerning transport currents

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The standard definition of a spin current, applied to the conductors lacking inversion symmetry, results in nonzero spin currents. I demonstrate that the spin currents do not vanish even in thermodynamic equilibrium, in the absence of external fields. These currents are dissipationless and are not associated with real spin transport. The result should be taken as a warning indicating problems inherent in the theory of transport spin currents driven by external fields.

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Generating spin currents (SC's) is one of the central goals of spintronics,¹ and various mechanisms for electrical and optical injection of SC's have been proposed. Recently, the interest in SC's has been strengthened by independent reports of dissipationless SC's in two different systems: holes in the valence band of a diamond-type crystal described by a Luttinger Hamiltonian² and electrons in a two-dimensional (2D) system with a structure inversion asymmetry (SIA) described by a Rashba Hamiltonian.³ These systems differ in symmetry because the Luttinger Hamiltonian possesses inversion symmetry while the Rashba Hamiltonian lacks it. In both cases, SC's are driven by an external electric field \mathbf{E} . Spin currents in a 3D Luttinger system are polarized perpendicularly to the driving field \mathbf{E} and the electron momentum \mathbf{k} .² In the 2D system of Ref. 3 they are polarized perpendicularly to the confinement plane (that contains both \mathbf{E} and \mathbf{k}). General properties of charge and spin transport in 2D systems with spin-orbit coupling have acquired intense attention lately.^{4,5}

The surprising results on dissipationless SC's have drawn a lot of attention, causing active interest and immediate response. They were followed by several papers of different researchers^{6–8} and also by the more recent papers coming from the same groups.^{9–11} The mathematical formalism in some of these papers, particularly in Refs. 2, 7, and 9, is rather involved. Meanwhile, the somewhat miraculous nature of the dissipationless SC's calls for a better understanding of their mechanism, including the properties of the background that supports the SC's linear in \mathbf{E} . From the standpoint of spintronic applications, it is important to understand whether these are *transport* currents, i.e., whether they can be employed for transporting spins, accumulating them at specific locations, and for injecting spins.

In this paper I am trying to contribute to this basic physical understanding. I consider noncentrosymmetric 2D systems in thermodynamic equilibrium and show that using the standard definition of a SC results in nonvanishing SC expectation value. This result is not entirely surprising from a general symmetry viewpoint. Indeed, the reversal of the momenta (or the velocities) only, without reversing the angular momenta (spins), cannot be reconciled with the time-inversion symmetry for noncentrosymmetric systems.¹² Of course, such *background* currents, which are present in the ground state in the absence of in-plane external fields, are nontransport currents.

The standard Hamiltonian with a Rashba term is

$$H_R = \hbar^2 k^2 / 2m + \alpha_R (\boldsymbol{\sigma} \times \mathbf{k}) \cdot \hat{\mathbf{z}}, \quad (1)$$

with $\boldsymbol{\sigma}$ the Pauli matrices, $\mathbf{k} = (k_x, k_y)$ the 2D momentum, and $\hat{\mathbf{z}}$ a unit vector perpendicular to the confinement plane. The eigenvalues of the Hamiltonian H_R are $E_\lambda(k) = \hbar^2 k^2 / 2m + \lambda |\alpha_R| k$, where $\lambda = \pm 1$ correspond to the upper and lower branches of the spectrum, respectively. The eigenfunctions are

$$\psi_\lambda(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i\lambda \alpha_R (k_x + ik_y) / |\alpha_R| k \end{pmatrix}. \quad (2)$$

The operator of the velocity is

$$\mathbf{v} = \hbar^{-1} \partial H_R / \partial \mathbf{k} = \hbar \mathbf{k} / m + \alpha_R (\hat{\mathbf{z}} \times \boldsymbol{\sigma}), \quad (3)$$

and the mean values of the Pauli matrices in the eigenstates $\psi_\lambda(\mathbf{k})$ are

$$\langle \boldsymbol{\sigma} \rangle_{\lambda \mathbf{k}} \equiv \langle \psi_\lambda(\mathbf{k}) | \boldsymbol{\sigma} | \psi_\lambda(\mathbf{k}) \rangle = \frac{\lambda \alpha_R}{|\alpha_R| k} (\mathbf{k} \times \hat{\mathbf{z}}). \quad (4)$$

These equations allow one to evaluate the SC components defined as products of the electron velocity and spin components.

For calculating SC's in a given state (λ, \mathbf{k}) , it is convenient to evaluate the Hermitian dot and cross products of $\boldsymbol{\sigma}$ and \mathbf{v} by using Eqs. (3) and (4):

$$\frac{1}{2} [(\boldsymbol{\sigma} \cdot \mathbf{v}) + (\mathbf{v} \cdot \boldsymbol{\sigma})] = \frac{\hbar}{m} (\boldsymbol{\sigma} \cdot \mathbf{k}), \quad \langle (\boldsymbol{\sigma} \cdot \mathbf{k}) \rangle_{\lambda \mathbf{k}} = 0$$

and

$$\frac{1}{2} \langle (\boldsymbol{\sigma} \times \mathbf{v}) - (\mathbf{v} \times \boldsymbol{\sigma}) \rangle_{\lambda \mathbf{k}} = \frac{\alpha_R}{\hbar} \left(2 + \lambda \frac{\hbar^2 k}{m |\alpha_R|} \right). \quad (5)$$

The dot product vanishes because the spin is polarized perpendicularly to \mathbf{k} in the eigenstates $\psi_\lambda(\mathbf{k})$. The Kramers conjugate states $\psi_\lambda(\mathbf{k})$ and $\psi_\lambda(-\mathbf{k})$ belong to the same branch of the spectrum. As a result, SC's of Eq. (5) are even with

respect to the change $\mathbf{k} \rightarrow -\mathbf{k}$ within each branch, while their values for different branches $\lambda = \pm 1$ are not mutually related. Therefore, there is no compensation of the SC's from different branches, and net macroscopic SC's can arise.

Electron spin is not conserved in the presence of a spin-orbit interaction because of precession in a momentum-dependent effective magnetic field. Therefore, the usual procedure for deriving currents from the continuity equations is not applicable to SC's (at least in its simplest form), and I use in what follows the standard and physically appealing definition of the SC tensor \mathcal{J}_{ij} :

$$\mathcal{J}_{ij} = \frac{1}{2} \sum_{\lambda} \int \frac{d^2k}{(2\pi)^2} \langle \sigma_i v_j + v_j \sigma_i \rangle_{\lambda k}. \quad (6)$$

Here $i, j = x, y$, with i indicating the spin component and j the transport direction. For $T=0$, the integration should be performed over $k \leq K_{\pm}$, where K_{\pm} are the Fermi momenta for both spectral branches. For the Hamiltonian H_R the tensor \mathcal{J}_{ij} is antisymmetric,

$$\mathcal{J}_{xx} = \mathcal{J}_{yy} = 0, \quad \mathcal{J}_{xy} = -\mathcal{J}_{yx} \equiv \mathcal{J}_R. \quad (7)$$

This tensor is invariant under the operations of the symmetry group $C_{\infty v}$ of the Hamiltonian H_R .

When the electrochemical potential μ is positive, $\mu > 0$, both spectral branches are populated and

$$\mathcal{J}_R(\mu) = m^2 \alpha_R^3 / 3\pi \hbar^5. \quad (8)$$

Therefore, the SC is odd in the coupling constant α_R , it is of the third order in α_R , and does not depend on μ . According to Eq. (5), spin currents carried by individual electrons are linear in α_R . The current $\mathcal{J}_R(\mu)$ is of the third order in α_R because of the factor $(m\alpha_R/\hbar^2 k_F)^2$ that is acquired as a result of the integration over the equilibrium Fermi distribution. This factor comes from a partial cancelation of the contributions of the upper and lower spectrum branches. It is small for high electron concentrations.

For comparison, the spin-orbit energy found by averaging the second term of H_R is even in α_R ($\mu \geq 0$):

$$E_{so}(\mu) = -(4/3\pi)(m\alpha_R/\hbar^2)^2(m\alpha_R^2/\hbar^2 + 3\mu/2). \quad (9)$$

For small electron concentrations, when $\mu < 0$ and electrons populate only the lower branch of the spectrum,

$$\mathcal{J}_R(\mu) = \frac{m\alpha_R}{3\pi\hbar^3} \left(\frac{m\alpha_R^2}{\hbar^2} - \mu \right) \sqrt{1 + 2\frac{\mu\hbar^2}{m\alpha_R^2}}. \quad (10)$$

Equations (8) and (10) match smoothly at $\mu = 0$; a discontinuity exists only in the second derivative. Near the bottom of the spectrum, at $\mu = E_{\min} = -m\alpha_R^2/2\hbar^2$, $\mathcal{J}_{xy}(\mu)$ shows a square-root singularity. The nonanalytical behavior at these points emerges because of the spectrum singularities at $E = 0$ and $E = E_{\min}$ and is also known for different phenomena.¹³

The SC's of Eqs. (8) and (10) were found under the conditions of thermodynamic equilibrium. Therefore, they do

not describe any real transport of electron spins and cannot result in spin injection or accumulation. Calculating transport currents would require a modification of Eq. (6). Nevertheless, Eq. (7) provides some insight into the effect of spin-orbit interaction on an equilibrium electron system. A real (i.e., invariant under time inversion) antisymmetric pseudotensor \mathcal{J}_{ij} is equivalent to a real vector $\mathbf{P} \parallel \hat{\mathbf{z}}$. It has the symmetry of the normal electric field \mathbf{E}_{\perp} producing the SIA and can be related to the spin-orbit contribution to the response of 2D electrons to this field. Interestingly, electric fields generated by SC's in magnetic insulators were discussed by Meier and Loss.¹⁴ (Despite a similarity, both the origin and the scale of the effect are very different from the above.)

Calculating SC's driven by an in-plane field \mathbf{E} is beyond the scope of the present work. Nevertheless, we point out at a resemblance between the background SC's $\mathcal{J}_{xy} = -\mathcal{J}_{yx}$ of Eq. (7) produced by the field \mathbf{E}_{\perp} and the dissipationless SC's of Refs. 2 and 3. Applying a driving field \mathbf{E} to a diamond-type crystal violates its inversion symmetry and, therefore, can produce background currents. To obtain transport SC's, these background currents should be eliminated.

The symmetry of the tensor \mathcal{J}_{ij} depends on the specific choice of the spin-orbit interaction. When it originates from the bulk inversion asymmetry (BIA), the Hamiltonian includes a Dresselhaus spin-orbit term. In the principal cubic axes it reads

$$H_D = \hbar^2 k^2 / 2m + \alpha_D (\sigma_x k_x - \sigma_y k_y). \quad (11)$$

As distinct from H_R , H_D possesses only C_{2v} symmetry. As a result, the ordering of electron spins with respect to \mathbf{k} is quite different, and

$$\mathcal{J}_{xx} = -\mathcal{J}_{yy} = \mathcal{J}_D, \quad \mathcal{J}_{xy} = \mathcal{J}_{yx} = 0, \quad (12)$$

where $\mathcal{J}_D(\mu)$ can be found from $\mathcal{J}_R(\mu)$ of Eqs. (8) and (10) by the substitution $\alpha_R \rightarrow \alpha_D$. Therefore, Eq. (6) results in equilibrium SC's also for BIA systems.

Spin currents of Eqs. (7) and (12) were found for two different 2D systems. It has been shown in Ref. 15 that in a 1D system with a linear-in- k spin-orbit coupling [similar to that of Eq. (1)], SC's vanish in thermodynamic equilibrium. This fact makes difficult establishing any specific connection between the equilibrium SC's of this paper and the SC's in single-channel ring textures¹⁶ and electron Berry phases in single-channel rings of noncentrosymmetric materials.¹⁷

In conclusion, the standard procedure for calculating spin currents, when applied to noncentrosymmetric crystals, results in nonvanishing currents even under the conditions of thermodynamic equilibrium. For calculating transport spin currents, a procedure for eliminating the background currents should be devised.

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